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PECASE – First Principles Modeling of Mechanics and Chemistry of Materials

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14. ABSTRACT

Recent experiments on nanostructured materials, such as nanoparticles, nanowires, nanotubes, nanopillars, thin films, and nanocrystals have revealed a host of ‘‘ultra-strength” phenomena, defined by stresses in a material component generally rising up to a significant fraction > 1/10th of its ideal strength – the highest achievable stress of a defect-free crystal at zero temperature. While conventional materials deform or fracture at sample-wide stresses far below the ideal strength, rapid development of nanotechnology has brought about a need to understand ultra-strength phenomena, as nanoscale materials apparently have a larger dynamic range of sustainable stress (‘‘strength”) than conventional materials. Ultra-strength phenomena not only have to do with the shape stability and deformation kinetics of a component, but also the tuning of its physical and chemical properties by stress. Reaching ultrastrength enables ‘‘elastic strain engineering”, where by controlling the elastic strain field one achieves desired electronic, magnetic, optical, phononic, catalytic, etc. properties in the component, imparting a new meaning to Feynman’s statement ‘‘there’s plenty of room at the bottom”.

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Final Report for PECASE FA9550-08-1-0325
First-principles modeling of mechanics and chemistry of materials

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Abstract

Recent experiments on nanostructured materials, such as nanoparticles, nanowires, nanotubes, nanopillars, thin films, and nanocrystals have revealed a host of ‘‘ultra-strength” phenomena, defined by stresses in a material component generally rising up to a significant fraction > 1/10th of its ideal strength – the highest achievable stress of a defect-free crystal at zero temperature. While conventional materials deform or fracture at sample-wide stresses far below the ideal strength, rapid development of nanotechnology has brought about a need to understand ultra-strength phenomena, as nanoscale materials apparently have a larger dynamic range of sustainable stress (‘‘strength”) than conventional materials. Ultra-strength phenomena not only have to do with the shape stability and deformation kinetics of a component, but also the tuning of its physical and chemical properties by stress. Reaching ultrastrength enables ‘‘elastic strain engineering”, where by controlling the elastic strain field one achieves desired electronic, magnetic, optical, phononic, catalytic, etc. properties in the component, imparting a new meaning to Feynman’s statement ‘‘there’s plenty of room at the bottom”. We are investigating the principal deformation mechanisms of ultra-strength materials. The fundamental defect processes that initiate and sustain plastic flow and fracture, and the mechanics and physics of both displacive and diffusive mechanisms are being modeled at the atomistic and electronic-structure levels. Also, electrochemistry coupled with mechanics dictates the microstructural evolution and service life of many materials, and underlies problems such as stress-corrosion cracking and battery cyclability. While atomistic and first-principles modeling is adept at looking at the finer details of energetics and microstructural evolution, it often needs help from experiments to identity the key performance-limiting microstructural processes. To resolve this bottleneck we have created a nanoscale electrochemical testing platform inside a transmission electron microscope (TEM), and performed direct observations of the electrochemical reactions of the individual nanowires. SnO_2, ZnO, Si, Ge, graphene and carbon nanotube anodes and $LiFePO_4$ nanowire cathode have been tested so far. Lithium embrittlement is found to be a persistent issue. These in situ TEM experiments greatly complement our modeling efforts, and together they provide unprecedented details on how materials degrade in service due to combined electrochemical-mechanical actions.

Fundind History

This PECASE award was initially granted to the PI at Ohio State University as FA9550-07-1-0007. Only $25,916 was spent out of the $500,000 budget, before the project was transferred to

the University of Pennsylvania as FA9550-08-1-0325, with a total budget of $474,083, and budget dates of May 1, 2008 - Nov. 30, 2012.

Results

The PI used the PECASE grant to perform a range of research activities on first-principles modeling of mechanics and chemistry of materials, in combination with critical experiments such as *in situ* electron microscopy. The publications supported by FA9550-08-1-0325 are listed in[1-30] in order of relevance for the high-temperature materials program. These work can be roughly categorized into the following:

Simulation of Coupled Displacive-Diffusional Processes – In the majority of solid-state processes, coupled displacive-diffusional processes is a rule rather than an exception. Mechanistic studies of these processes require modeling capabilities at atomistic length scales but diffusional time scales, which is beyond the reach of current molecular dynamics (MD) methods. Partially supported by this project, a new computational method called Diffusive Molecular Dynamics (DMD) is being developed[1], which, unlike the MD, captures diffusional and displacive evolution of complex microstructures at the atomic scale by coarse graining over atomic vibrations and evolving a continuous occupational probability of atomic density clouds. Derived in grand canonical ensemble, DMD is a chemical mean-field extension of the variational Gaussian method coupled with the master equation for diffusion solved on a discrete and moving atomic grid. It combines long-range elastic effects and short-range atomic interactions simultaneously with gradient thermodynamics and allows for simultaneous displacive and mass-action dynamics such as lattice diffusion. We are also developing corresponding phase-field descriptions of these transformations, which eventually could seamlessly link to DMD as in the quasi-continuum approach.

Studying Slow Dynamics - In order to study the slow dynamics in glassy materials[30] in general, we have developed a Markovian network model to calculate the shear viscosity of deeply supercooled liquids based on sampling of an atomistic energy landscape. Shear stress relaxation is calculated from a master-equation description in which the system follows a transition-state pathway trajectory of hopping among local energy minima separated by activation barriers, which is in turn sampled by accerlated MD-based algorithms[6]. Quantitative connection is established between the temperature variation of the calculated viscosity and the underlying potential energy and inherent stress landscape of several glasses[11,12], showing a different landscape topography or 'terrain' is needed for low-temperature viscosity from that associated with high-temperature viscosity[11]. We have also developed an accerlated 'strain-boost' MD algorithm[6], inspired by the Eshelby transformation formalism, that could provide more effecicient sampling of the shear transformation zone (STZ) event in glasses.

In particular, silica (SiO_2) glass is one of the essential materials in human civilization for making household items, window panes, lenses and optical fibers. An important reason for its wide adaptation is its formability near the glass-transition temperature (T_g > 1100C). SiO_2 glass at room temperature, however, is usually brittle due to fracture instability. But when the "brittle" glass is confined in extremely small dimensions at tens of nanometres, the nature of flow and fracture may change. Newest experiments performed at Sandia Center for Integrated Nanotechnologies (CINT) show that glass nanowires with diameters less than 20 nm can become ductile at room temperature, with surprisingly large tensile plastic elongations up to 18%. Remarkably, these ductile glass nanowires also possess high flow strengths, and are thus much more energy-absorbing and damage-tolerant than expected. Atomistic modeling indicates that the unexpected ductility is due to the development of a surface affected zone in the nanowires, which enhances ductility by producing more bond-switching events per irreversible bond loss.

Investigating Solid-state Amorphization Processes - We have studied the solid-state amorphization of phase-change nanowires[4] and large shape change of oxide nanowires during electrochemical lithiation, which share certain common characteristics with strain glasses (both solid-state, and both with significant transformation strains). We found that upon electrochemical charging, a reaction front propagated progressively along the nanowire, causing the nanowire to swell, elongate, and spiral. The reaction front contains a high density of mobile dislocations, which are continuously nucleated and absorbed at the moving front. This dislocation cloud indicates large in-plane misfit stresses and is a structural precursor to electrochemically driven solid-state amorphization. Because amorphization-induced volume expansion, plasticity, and pulverization of electrode materials are the major mechanical effects that plague the performance and lifetime of high-capacity anodes in lithium-ion batteries, our observations provide important mechanistic insight for the design of advanced batteries, as well as damage mechanisms in strain glasses. In the modeling effort we have also given a first-principles account of the observed room-temperature lithium diffusivity in amorphous lithium oxide[5].

High-temperature sublimation of graphene – We have performed in situ transmission electron microscopy (TEM) and modeling of how graphene sublimes at high temperatures. Curvy nanostructures such as carbon nanotubes and fullerenes have extraordinary properties but are difficult to pick up and assemble into devices after synthesis. We have performed experimental and modeling research into how to integrate curvy nanostructures on flat graphene, taking advantage of the fact that graphene bends easily after open edges have been cut on it, which can then fuse with other open edges, like a plumber connecting metal fittings. By applying electrical current heating to few-layer graphene inside an electron microscope, one effectively anneals out the radiation damage and observes the *in situ* creation of many interconnected, curved carbon nanostructures[7], such as graphene bilayer edges (BLEs) aka "half nanotubes", BLE polygons, and nanotube-BLE junctions connecting multiple layers of graphene. A novel piezoelectric effect causes the BLEs to have large permanent electric dipoles of 0.87 and 1.14 Debye/Å for zigzag and armchair inclinations, respectively[10]. Unlike carbon nanotubes which fold graphene by 2π rotation and are highly poly-disperse in chiralities and radius, BLEs are highly mono-disperse

structures due to the π rotation and a lattice orientation constraint during processing[3]. Further investigations indicate that multiple-layer graphene offers unique opportunities for tailoring carbon-based structures and engineering novel nano-devices with complex topologies. In particular, we show it is possible to create a metal-semiconductor-metal graphene-nanotube junction device with 0.8eV electronic gap[9].

Nanoscale electrochemical tests: in situ TEM experiments and modeling - Electrochemistry coupled with mechanics dictates the microstructural evolution and service life of many materials in the energy industry and transportation, and underlies problems such as stress-corrosion cracking and battery cyclability. While atomistic and first-principles modeling is adept at looking at the finer details of energetics and microstructural evolution, it often needs help from experiments to identity the key performance-limiting microstructural processes. To resolve this bottleneck we have created a nanoscale electrochemical testing platform[2,5] inside a transmission electron microscope (TEM), consisting of electron-transparent single nanowire electrodes and an ionic liquid electrolyte, and performed direct observations of the electrochemical reactions of the individual nanowires. SnO2, ZnO, Si, Ge, graphene and carbon nanotube anodes and $LiFePO_4$ nanowire cathode have been tested so far. Lithium embrittlement is found to be a persistent issue. These in situ TEM experiments[13,28] greatly complement our modeling efforts[1,6,9,11], and together they provide unprecedented details on how materials degrade in service due to combined electrochemical-mechanical actions.

Utra-strength materials - Recent experiments on nanostructured materials, such as nanoparticles, nanowires, nanotubes, nanopillars, thin films, and nanocrystals have revealed a host of ‘‘ultra-strength” phenomena, defined by stresses in a material component generally rising up to a significant fraction > 1/10th of its ideal strength – the highest achievable stress of a defect-free crystal at zero temperature. While conventional materials deform or fracture at sample-wide stresses far below the ideal strength, rapid development of nanotechnology has brought about a need to understand ultra-strength phenomena, as nanoscale materials apparently have a larger dynamic range of sustainable stress (‘‘strength”) than conventional materials. Ultra-strength phenomena not only have to do with the shape stability and deformation kinetics of a component, but also the tuning of its physical and chemical properties by stress. Reaching ultrastrength enables ‘‘elastic strain engineering”, where by controlling the elastic strain field one achieves desired electronic, magnetic, optical, phononic, catalytic, etc. properties in the component, imparting a new meaning to Feynman’s statement ‘‘there’s plenty of room at the bottom”. We are investigating the principal deformation mechanisms of ultra-strength materials. The fundamental defect processes that initiate and sustain plastic flow and fracture, and the mechanics and physics of both displacive and diffusive mechanisms are being modeled at the atomistic and electronic-structure levels.[8,13,28]

Elastic Strain Engineering – An optoelectronic material with a spatially varying bandgap that is tunable is highly desirable for use in photovoltaics, photocatalysis and photodetection. Elastic

strain has the potential to be used to achieve rapid and reversible tuning of the bandgap. However, as a result of plasticity or fracture, conventional materials cannot sustain a high enough elastic strain to create sufficient changes in their physical properties. Recently, an emergent class of materials—named 'ultrastrength materials'—have been shown to avoid inelastic relaxation up to a significant fraction of their ideal strength. In the paper "Strain-engineered artificial atom as a broad-spectrum solar energy funnel" [29], we illustrate theoretically and computationally that elastic strain is a viable agent for creating a continuously varying bandgap profile in an initially homogeneous, atomically thin membrane. We propose that a photovoltaic device made from a strainengineered MoS_2 monolayer will capture a broad range of the solar spectrum and concentrate excitons or charge carriers.

Acknowledgments/Disclaimer

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Awards Received

TMS Robert Lansing Hardy Award (2009), for "a young person in the broad fields of metallurgy and materials science for exceptional promise of a successful career".

German-American Frontiers of Engineering Symposium (Oak Ridge, April 22-25, 2010) cosponsored by National Academy of Engineering and the Alexander von Humboldt Foundation.

Chinese Ministry of Education and Li Ka Shing Foundation Chang Jiang Scholar Award (2009)

Technology Review TR35 award, for 35 "world's top innovators" under age 35 (2007)

Best Poster Award, Gordon Research Conferences on Physical Metallurgy, August 2-7, 2009, Proctor Academy, Andover, NH: Erik Bitzek, William T. Cox, Sanket Sarkar, Thomas J. Lenosky, Yunzhi Wang, Ju Li, "Atomic-Scale Modeling of Diffusion-Driven Microstructure Evolution".

Presentations

Invited talk, 2012 MRS Fall Meeting, Boston, November 27, 2012.

Plenary talk, "Diffusive Molecular Dynamics (DMD): Simulating Displacive-Diffusive Transformations without Tracking Billions of Hops," Multiscale Materials Modeling (MMM) 2012 conference, October 15-19, Biopolis, Singapore.

Invited talk, Nanoscale Science and Engineering Seminar Series, University of California at Berkeley, April 13, 2012.

Invited talk, 2012 MRS Spring Meeting, San Francisco, April 9-13, 2012.

Keynote talk, TMS 2012 Annual Meeting & Exhibition, Orlando, March 11-15, 2012.

Invited talk, APS March Meeting, Boston, February 27-March 2, 2012.

Invited talk, Plasticity 2012, San Juan, Puerto Rico, January 3-8, 2012.

Joint MIT ANS Student Chapter / faculty seminar on "Nanoscale electrochemical tests: in situ TEM experiments and modeling", November 21, 2011.

First Annual Richard K. Osborn Lecture, Department of Nuclear Engineering and Radiological Sciences, University of Michigan, Stamps Auditorium, September 23, 2011.

Lee Hsun Young Scientist Lecture Series on Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang, China, July 18, 2011.

Keynote presentation, ASME McMat2011, symposium on Low Dimensional Carbon NanoMaterials: Properties and Applications, Chicago, May 31-June 2, 2011.

Invited talk, Electron Microscopy and Multiscale Modeling 2011, Granlibakken Conference Center and Lodge, May 22-27, 2011.

Invited talk, Pennergy Symposium "Materials Under Extremes," April 9, 2011, Philadelphia.

Invited talk, Harvard Applied Mechanics Colloquium, February 2, 2011.

Invited talk, MRS Fall Meeting, Boston, November 29 - December 3, 2010.

Microstructure Modelling symposium, MMM2010, the Fifth Conference on Multiscale Material Modelling, Freiburg, Germany, October 7, 2010.

Penn Department of Mechanical Engineering and Applied Mechanics Seminar Series, September 16, 2010.

Invited talk, Physics and Astronomy Colloquium Series at University of Southern California, August 30, 2010.

Invited talk, Department of Engineering Science and Mechanics, Pennsylvania State University, July 16, 2010.

Invited talk, 17th International Symposium on Metastable, Amorphous and Nanostructured Materials (ISMANAM 2010), Zurich, Switzerland, July 4 - 9, 2010.

Invited talk, Sixth International Conference on Materials Structure & Micromechanics of Fracture (MSMF6), Brno, Czech Republic, June 28 - 30, 2010.

Invited talk, Department Werkstoffwissenschaften, Lehrstuhl WWI: Allgemeine Werkstoffeigenschaften, Universitat Erlangen-Nurnberg, Germany, June 24, 2010.

Invited talk, International Workshop on Materials Behavior at Micro- and Nano-Scale, Xi'an, China, June 11, 2010.

Invited talk, International Conference on Mechanical Properties of Materials (ICMPM), Hangzhou, China, May 27, 2010.

Two invited talks, 2010 SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, May 23, 2010.

Invited talk, Materials Science and Engineering Seminar, University of Tennessee, Knoxville, April 26, 2010.

Invited talk, Materials Science and Engineering Seminar, Rensselaer Polytechnic Institute, Troy, April 7, 2010.

Invited talk, TMS 2010 Annual Meeting & Exhibition, Seattle, February 14-18, 2010.

Keynote talk (40 min), mini-symposium Finite Plasticity & Viscoplasticity of Conventional & Emerging Materials (In celebration of 65 Years of Akhtar Khan), Plasticity 2010, St. Kitts, West Indies, January 3-8, 2010.

Invited talk, MIT Center for Computational Engineering (CCE), December 2, 2009.

Invited talk, MRS Fall Meeting, symposium Mechanical Behavior of Nanomaterials Experiments and Modeling, Boston, November 30 - December 4, 2009.

Invited talk, Civil Infrastructure Seminar, School of Civil and Environmental Engineering, Cornell University, November 10, 2009.

Invited talk, Mechanical & Aerospace Engineering Seminar, The University of Texas at Arlington, September 4, 2009.

Invited talk, Department of Mechanical Engineering Seminar, University Of Houston, September 3, 2009.

Invited talk, Workshop on Probing the Limits of Strength, Lawrence Berkeley National Laboratory, Berkeley, California, August 11-12, 2009.

Invited talk, "In-situ Observation of Graphene Sublimation and Edge Reconstructions," mini-symposium Graphene growth and properties through experiments and simulations, tenth U.S. National Congress on Computational Mechanics (USNCCM X), Columbus, July 16-19, 2009.

Invited talk, School of Materials Science and Engineering, Shanghai Jiao Tong University, June 10, 2009.

Invited talk, International Workshop on Size Effect on Materials Mechanical Behavior, Beijing, May 24 - 26, 2009.

Invited talk, "The Coming of Age of Ultra-Strength Materials," Center for Integrated Nanotechnologies (CINT), Sandia National Laboratories, Albuquerque, New Mexico, May 7, 2009.

Invited talk, Othmer-Jacobs Department of Chemical and Biological Engineering, Polytechnic Institute of NYU, Brooklyn, New York, May 4, 2009.

Invited talk, MRS Spring Meeting, symposium Probing Mechanics at Nanoscale Dimensions, San Francisco, April 13-17, 2009.

Invited talk, Shanghai Institute of Ceramics, March 10, 2009.

Invited talk, TMS 2009 Annual Meeting & Exhibition, San Francisco, February 15-19, 2009.

Keynote talk (40 min), "Tensile Ductility of Nanostructured Metals," Plasticity 2009, St. Thomas, U.S. Virgin Islands, January 3-8, 2009.

Invited talk, Workshop on Mechanical Behaviors of Micro/Nano Materials, XiAn Jiao Tong University, December 30-31, 2008.

Two invited talks, National Sun Yat-sen University, Kaohsiung, Taiwan, December 13-21, 2008.

Invited talk, Georgia Institute of Technology Woodruff School of Mechanical Engineering Seminar, Oct. 23, 2008.

Invited talk, Dislocations 2008, Hong Kong, Oct. 13-17, 2008.

Invited talk, Brown University Joint Materials/Solid Mechanics Seminar, September 12, 2008.

Invited talk, "Plasticity in amorphous and nanocrystalline metals," Gordon Research Conference on Thin Film & Small Scale Mechanical Behavior, Colby College, Maine, July 27 - August 1, 2008.

Two invited lectures, Workshop on Multi-Scale Modeling of Moving Interfaces in Materials, Katholieke Universiteit Leuven, Belgium, July 2-4, 2008.

Invited talk, 2nd International Conference on Heterogeneous Materials Mechanics (ICHMM-2008), HuangShan, China, June 3-8, 2008.

Invited talk, International Workshop on in situ Electron Microscopy in Advanced Materials Research, Beijing, May 31 - June 2, 2008.

Invited talk, NIST 2008 Diffusion Workshop, Gaithersburg, Maryland, May 12-13, 2008.

Publications acknowledging AFOSR support, ranked in order of relevance for the high-temperature materials program; Li, J. means being a corresponding author

1. J. Li, S. Sarkar, W. T. Cox, T. J. Lenosky, E. Bitzek & Y. Z. Wang. Diffusive molecular dynamics and its application to nanoindentation and sintering. *Phys. Rev. B* **84**, 054103 (2011).

2. A. Kushima, X. H. Liu, G. Zhu, Z. L. Wang, J. Y. Huang & J. Li. Leapfrog Cracking and Nanoamorphization of ZnO Nanowires during In Situ Electrochemical Lithiation. *Nano Lett.* **11**, 4535-4541 (2011).

3. L. Qi, J. Y. Huang, J. Feng & J. Li. In situ observations of the nucleation and growth of atomically sharp graphene bilayer edges. *Carbon* **48**, 2354-2360 (2010).

4. S. W. Nam, H. S. Chung, Y. C. Lo, L. Qi, J. Li, Y. Lu, A. T. C. Johnson, Y. W. Jung, P. Nukala & R. Agarwal. Electrical Wind Force-Driven and Dislocation-Templated Amorphization in Phase-Change Nanowires. *Science* **336**, 1561-1566 (2012).

5. J. Y. Huang, L. Zhong, C. M. Wang, J. P. Sullivan, W. Xu, L. Q. Zhang, S. X. Mao, N. S. Hudak, X. H. Liu, A. Subramanian, H. Y. Fan, L. A. Qi, A. Kushima & J. Li. In Situ Observation of the Electrochemical Lithiation of a Single SnO(2) Nanowire Electrode. *Science* **330**, 1515-1520 (2010).

6. S. Hara & J. Li. Adaptive strain-boost hyperdynamics simulations of stress-driven atomic processes. *Phys. Rev. B* **82**, 184114 (2010).

7. J. Y. Huang, F. Ding, B. I. Yakobson, P. Lu, L. Qi & J. Li. In situ observation of graphene sublimation and multi-layer edge reconstructions. *PNAS* **106**, 10103-10108 (2009).

8. T. Zhu & J. Li. Ultra-strength materials. *Prog. Mater Sci.* **55**, 710-757 (2010).

9. J. S. Qi, J. Y. Huang, J. Feng, D. N. Shi & J. Li. The Possibility of Chemically Inert, Graphene-Based All-Carbon Electronic Devices with 0.8 eV Gap. *ACS Nano* **5**, 3475-3482 (2011).

10. J. Feng, L. Qi, J. Y. Huang & J. Li. Geometric and electronic structure of graphene bilayer edges. *Phys. Rev. B* **80**, 165407 (2009).

11. J. Li, A. Kushima, J. Eapen, X. Lin, X. F. Qian, J. C. Mauro, P. Diep & S. Yip. Computing the Viscosity of Supercooled Liquids: Markov Network Model. *Plos One* **6**, e17909 (2011).

12. A. Kushima, J. Eapen, J. Li, S. Yip & T. Zhu. Time scale bridging in atomistic simulation of slow dynamics: viscous relaxation and defect activation. *European Physical Journal B* **82**, 271-293 (2011).

13. Q. Yu, Z. W. Shan, J. Li, X. X. Huang, L. Xiao, J. Sun & E. Ma. Strong crystal size effect on deformation twinning. *Nature* **463**, 335-338 (2010).

14. J. Y. Huang, L. Qi & J. Li. In Situ Imaging of Layer-by-Layer Sublimation of Suspended Graphene. *Nano Res.* **3**, 43-50 (2010).

15. Y. Mishin, M. Asta & J. Li. Atomistic modeling of interfaces and their impact on microstructure and properties. *Acta Mater.* **58**, 1117-1151 (2010).

16. N. Zhou, C. Shen, M. J. Mills, J. Li & Y. Z. Wang. Modeling displacive-diffusional coupled dislocation shearing of gamma ' precipitates in Ni-base superalloys. *Acta Mater.* **59**, 3484-3497 (2011).

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18. X. H. Liu, S. Huang, S. T. Picraux, J. Li, T. Zhu & J. Y. Huang. Reversible Nanopore Formation in Ge Nanowires during Lithiation-Delithiation Cycling: An In Situ Transmission Electron Microscopy Study. *Nano Lett.* **11**, 3991-3997 (2011).

19. Y. Liu, H. Zheng, X. H. Liu, S. Huang, T. Zhu, J. W. Wang, A. Kushima, N. S. Hudak, X. Huang, S. L. Zhang, S. X. Mao, X. F. Qian, J. Li & J. Y. Huang. Lithiation-Induced Embrittlement of Multiwalled Carbon Nanotubes. *ACS Nano* **5**, 7245-7253 (2011).

20. S. Ogata & J. Li. Toughness scale from first principles. *J. Appl. Phys.* **106**, 113534 (2009).

21. S. Z. Li, X. D. Ding, J. K. Deng, T. Lookman, J. Li, X. B. Ren, J. Sun & A. Saxena. Superelasticity in bcc nanowires by a reversible twinning mechanism. *Phys. Rev. B* **82**, 205435 (2010).

22. S. Z. Li, X. D. Ding, J. Li, X. B. Ren, J. Sun & E. Ma. High-Efficiency Mechanical Energy Storage and Retrieval Using Interfaces in Nanowires. *Nano Lett.* **10**, 1774-1779 (2010).

23. S. Z. Li, X. D. Ding, J. Li, X. B. Ren, J. Sun, E. Ma & T. Lookman. Inverse martensitic transformation in Zr nanowires. *Phys. Rev. B* **81**, 245433 (2010).

24. X. H. Liu, L. Zhong, L. Q. Zhang, A. Kushima, S. X. Mao, J. Li, Z. Z. Ye, J. P. Sullivan & J. Y. Huang. Lithium fiber growth on the anode in a nanowire lithium ion battery during charging. *Appl. Phys. Lett.* **98**, 183107 (2011).

25. X. F. Qian, J. Li & S. Yip. Calculating phase-coherent quantum transport in nanoelectronics with ab initio quasiatomic orbital basis set. *Phys. Rev. B* **82**, 195442 (2010).

26. H. Y. Yuan, C. J. Huang, J. Li, G. Lykotrafitis & S. L. Zhang. One-particle-thick, solvent-free, coarse-grained model for biological and biomimetic fluid membranes. *Phys. Rev. E* **82**, 011905 (2010).

27. J. Y. Zhang, G. Liu, R. H. Wang, J. Li, J. Sun & E. Ma. Double-inverse grain size dependence of deformation twinning in nanocrystalline Cu. *Phys. Rev. B* **81**, 172104 (2010).

28. L. Huang, Q.-J. Li, Z.-W. Shan, J. Li, J. Sun & E. Ma. A new regime for mechanical annealing and strong sample-size strengthening in body centred cubic molybdenum. *Nat Commun* **2**, 547 (2011).

29. J. Feng, X. F. Qian, C. W. Huang & J. Li. Strain-engineered artificial atom as a broad-spectrum solar energy funnel. *Nature Photon.* **6**, 865-871 (2012).

30. P. Y. Zhao, J. Li & Y. Z. Wang. Heterogeneously randomized STZ model of metallic glasses: Softening and extreme value statistics during deformation. *Int. J. Plast.* **40**, 1-22 (2013).